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Radiological Health

A COMPUTER PROGRAM FOR THE ANALYSIS OF GAMMA-RAY SPECTRA BY THE METHOD OF LEAST SQUARES

U. S. DEPARTMENT OF HEALTH, EDUCATION, AND WELFARE

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A COMPUTER PROGRAM FOR THE ANALYSIS OF GAMMA-RAY SPECTRA BY THE METHOD OF LEAST SQUARES

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ACKNOWLEDGMENT

The authors express their appreciation to Dr. R. J. Augustine and Mr. Roger H. Schneider whose helpful suggestions were incorporated in the program.

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ABSTRACT

A computer program, written in Fortran II and Fortran IV languages for the IBM 1620 and 7040-1401 computers, respectively, is presented for the analysis of gamma-ray spectra by the method of least squares. The Fortran IV main program and four subroutines are included in appendices. The method is accurate, agreeing favorably with estimated standard deviations, and is sufficiently sensitive to be useful for routine analysis of gamma-ray spectra of a substantial number of low-activity samples. Data provided by a verification experiment show that the least squares method is more accurate than the simultaneous equations method.

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A COMPUTER PROGRAM FOR THE ANALYSIS OF GAMMA-RAY SPECTRA BY THE METHOD OF LEAST SQUARES

INTRODUCTION

With increasing numbers of projects for the assessment of radionuclide levels in man's environment, multichannel gamma-ray spectrometers have become of prime importance. The spectrometers offer an expeditious method, requiring minimal sample preparation, for the evaluation of gamma-ray emitting radionuclide levels in environmental media. To further facilitate the analysis of such samples, it is desirable to analyze the gamma-ray spectra by electronic data processing methods.

The least squares analysis of gamma-ray spectra is more accurate than other methods and makes maximum use of the resolution of the sodium iodide detector, as pointed out by Salmon (*1*). The method is readily adaptable to computer analysis and presents parameters by which the accuracy of the unfolding of the spectra can be evaluated.

This report presents a computer program for the analysis of gamma-ray spectra of environmental media by the method of least squares. A thorough discussion of the least squares prineiple as it applies to gamma spectrum analysis has been published elsewhere (*1-3*).

Because of the low activity and corresponding relatively large statistical fluctuations usually associated with environmental media, there is debate as to the best approach to the least squares solution. In this study the experimental verification of the validity of the least squares method was attempted, and certain techniques which might yield satisfactory solutions in these less than ideal situations were considered.

The program is written in the Fortran II and Fortran IV languages for the IBM 1620 (60,000 bit memory) and 7040-1401, respectively. Appendix A contains the Fortran IV main program. Appendix B contains four subroutines in the main program. The appendices are included for those who wish to use this program directly.

THEORETICAL DEVELOPMENT

LEAST SQUARES THEORY

The following symbols are used in describing the theory and the program:

Symbol	Definition
Y_o	Observed sample count in any one channel
Y_c	Computed sample count in any one channel corresponding to an observed count
δ	The actual deviation in counts $(Y_o - Y_c)$
σ	The standard deviation in a particular channel $(\sqrt{Y_o})$
δ_σ	The deviation (δ) in σ units
n	Number of channels analyzed
m	Number of standards

THE EQUATION OF CONDITION

The sample spectrum is assumed to be some linear combination of known standard spectra, and the equation of condition (for any one channel) is:

$$Y_c = a_1x_1 + a_2x_2 + \cdots + a_mx_m$$

where the a's are the unknown concentrations of the standard nuclides x_1, x_2, . . . up to x_m. This is a true physical model if the instrument is linear over the range of activities considered and if there is no variation in instrument response during the course of all observations.

LEAST SQUARES PRINCIPLE

The application of the least squares principle should yield the best estimates of the concentrations of the components if:

(1) the equation of condition is a true representation of the physical effects observed;

(2) the variance in the standards is negligible compared to that in the sample; and

(3) the fluctuation in the observations is distributed normally with common variance.

The least squares solution yields a set of coefficients (concentrations as fractions of the standard concentrations) that minimizes the following sum over all channels analyzed:

$$\sum_{i=1}^{n} w \cdot \delta_i^2$$

where w is the weight given to a particular channel. When w is defined as $1/Y_o$—a weighting procedure which gives the required common variance to all observations—then:

$$\Sigma \frac{1}{Y_o} \cdot \delta^2 = \Sigma \frac{1}{\sigma^2} \cdot \delta^2 = \Sigma \delta_\sigma^2.$$

Thus, weighting in this manner changes the minimization problem from that of minimizing the sum of squares of actual count residuals to minimizing the sum of squares of residuals in standard deviation units. However, giving the lowest counts the largest weights results in a computed spectrum which has fewer total counts than the observed spectrum. The computed spectrum is usually smoother than the observed spectrum, and, for this reason, Y_c is usually a more accurate estimate of the variance in an individual channel (*2*). An iterative scheme can be developed by repeating the least squares solution, using $1/Y_c$ as a weighting factor. Weighting by this factor brings the total counts in the computed spectrum into very close agreement with the observed spectrum.

Several "fit" parameters can be computed to determine the success of a particular solution. One of these, as suggested by Salmon (*1*), is the ratio:

$$R = \frac{X^2}{(n-m)} = \sum_{i=1}^{n} \frac{(Y_{oi} - Y_{ci})^2}{Y_{ci}} \; (n-m).$$

If R is significantly greater than unity, the standards either (1) do not represent all the nuclides present in the sample, (2) have not been counted for a sufficient length of time to make their statistical uncertainties insignificant compared to those of the sample, or (3) have not been measured at the same analyzer gain or threshold bias as the sample. In actual practice, R is almost always greater than 1, but the results can still be considered valid if the increase can be attributed to random errors (*1*).

As in any method of spectrum analysis, the analyzer gain and threshold bias must be controlled. The effects of changes of these two analyzer parameters are discussed by Schonfeld *et al.* (*4*). However, programs have been written that correct for small

changes in analyzer gain (*4,5*). It was not necessary to include such a feature in the program described as the gain was adequately controlled on the instruments utilized.

Data subjected to lease squares fitting should satisfy the requirement that errors of observations follow the Gaussian error curve, as pointed out earlier in this report. Thus, the errors in the standard deviation unit (δ_σ) should have a zero mean and unity variance. The latter two parameters are also a measure of the "goodness of fit."

PROGRAM FEATURES

Allowance for background is made by either of two methods. Background can be subtracted from each sample spectrum prior to the least squares solution, or it can be treated as the standard; that is, as a statistical variable in the least squares solution. Routinely the latter is used in this program.

In the first least squares solution of a sample spectrum, weights by the reciprocals of the observed counts ($1/Y_o$) are used. As stated earlier, this produces a computed spectrum with a low bias. Then, the least squares solution is repeated, weighting by the reciprocals of the computed counts ($1/Y_c$). This process can be repeated as many times as desired. However, little advantage has been noted after the first repetition.

The program contains provisions for obtaining a simultaneous equations solution (*6*). This has no relation to the least squares solution. However, to compare results obtained by the two methods, the simultaneous equations solution was included in developing the program and was retained in the final program.

An example of the output information obtained from the Fortran IV program is shown below. Copies of the input data format are available on request.

EXPERIMENTAL VERIFICATION

Each sample was counted in a 3.5-liter Marinelli beaker by a multichannel pulse height analyzer for 50 minutes. The detector was a cylindrical sodium iodide, thallium-activated crystal with dimensions of 4- by 4-inches.

Table 1 shows the results of least squares analyses of six spectra of samples containing a known amount of activity. The "known" samples were prepared from standard solutions whose activities

Example of output information obtained from the Fortran IV program

Standards Considered:

34 42310	BG
33 42314	^{131}I
33 42312	^{137}Cs
33 42311	K
33 42313	$^{140}Ba\text{-}La$

Samples:

Sample Number 31 42314 603

	BG	^{131}I pCi/l	^{137}Cs pCi/l	K gm/l	$^{140}Ba\text{-}La$ pCi/l
Computed Activity:	1.026	84.771	172.832	1.526	0.0
Standard Deviation:	0.026	1.070	7.452	0.087	0.0

$\sum_{i=1}^{n} Y_{oi}$ = 24767. $\sum_{i=1}^{n} Y_{ci}$ = 24767. $\sum_{i=1}^{n} w.\delta_i^2$ = 0.82388672E 02

R = 0.11442871E 01 $\sum_{i=1}^{n} \delta_i^2$ = 0.95318383E 05

n = 95 mean of the errors (δ_σ) = -0.048 standard deviation of errors (δ_σ) = 1.068

Channel Number	Y_o	$\sqrt{Y_o} = \sigma$	Y_c	δ	$\delta\sigma$
4	984.000	31.368	966.545	17.454	.5
5	1177.000	34.307	1160.489	16.510	.4
6	809.000	28.442	826.484	-17.484	-.6
7	1668.000	40.841	1661.022	6.977	.1
8	1897.000	43.554	1904.024	-7.024	-.1
9	2094.000	45.760	2147.917	-53.917	-1.1
10	2066.500	45.458	2076.091	-9.591	-.2
11	1804.000	42.473	1805.099	-1.099	0.0
12	1556.500	39.452	1519.708	36.791	.9
13	1349.500	36.735	1364.878	-15.378	-.4
14	1242.500	35.249	1297.486	-54.986	-1.5
15	1390.500	37.289	1323.623	66.876	1.7
16	1205.000	34.713	1246.564	-41.564	-1.1
17	1176.500	34.300	1156.390	20.109	.5
18	2049.500	45.271	1993.786	55.713	1.2
19	3603.500	60.029	3492.623	110.876	1.8
20	2954.000	54.350	3058.048	-104.048	-1.9

Table 1. Results of least squares analyses compared to simultaneous equations analyses

Sample number	Nuclide	Actual activity (pCi)	Least square analysis			Simultaneous equations analysis	
			Computed activity (pCi)	Error percent	Standard deviation percent	Computed activity (pCi)	Error percent
1	^{131}I	370	380	2.7	3.3	340	8.1
	^{137}Cs	470	440	6.4	4.8	390	17.0
	^{106}Ru	540	450	16.6	19.0	660	22.2
2	^{95}Zr	610	550	9.8	4.4	540	11.5
	^{54}Mn	540	680	25.9	3.8	600	11.1
	^{144}Ce	390	360	7.7	21.2	370	5.1
	^{65}Zn	340	350	2.9	9.5	390	14.7
3	^{131}I	740	730	1.4	2.5	710	4.1
	^{95}Zr	610	590	3.3	4.9	660	8.2
	^{54}Mn	1080	1150	6.5	2.9	1060	1.9
	^{22}Na	500	480	4.0	4.7	390	22.0
	^{65}Zn	690	670	2.9	6.6	710	2.9
4	^{137}Cs	950	920	3.2	4.3	980	3.2
	^{54}Mn	1080	1060	1.9	3.6	980	9.3
	^{60}Co	500	430	14.0	4.7	360	28.0
	^{144}Ce	790	730	7.6	17.8	900	15.2
	^{106}Ru	1090	1150	5.5	13.6	380	65.1
5	^{131}I	370	390	5.4	6.3	330	10.1
	^{137}Cs	470	440	6.4	9.5	640	36.2
	^{54}Mn	1090	1100	1.1	3.5	1100	0.92
	^{60}Co	1480	1400	5.4	2.8	1250	15.5
	^{22}Na	1990	2010	1.0	3.1	2280	14.6
	^{144}Ce	790	630	20.2	24.5	1080	36.7
	^{65}Zn	1380	1140	17.4	10.1	1540	11.6
	^{106}Ru	1640	1900	15.9	18.8	1530	6.7
6	^{131}I	1480	1450	2.0	2.2	1240	16.2
	^{137}Cs	470	450	4.3	10.8	330	29.8
	^{95}Zr	1830	1900	3.8	2.8	1920	4.9
	^{54}Mn	1620	1610	0.6	3.2	1520	6.2
	^{60}Co	990	1000	1.0	3.9	1010	2.2
	^{22}Na	1490	1430	4.0	4.5	1230	17.4
	^{65}Zn	340	380	12.0	28.0	330	2.9
	^{106}Ru	1090	1070	1.8	35.9	2220	103.3

were known with ±5 percent error. The results of the least squares analyses are compared with those obtained by the simultaneous equations solution.

Figures 1-4 are graphic examples of the analyses of the spectra of environmental and simulated environmental media. Simulated media were used because of the absence of fresh fission products in environmental media during the development of the program. Experimental points indicate points as taken from the pulse height analyzer data.

DISCUSSION and CONCLUSIONS

As shown in table 1, the results obtained by the least squares method are, in general, more accurate than those obtained by the simultaneous equations method. Salmon has shown that the least squares method is superior to the successive subtraction method, and is free of subjective errors (*1*). The least squares method utilizes all experimental data points, can be used for those nuclides whose photopeaks are superimposed, and presents standard deviations of the nuclide concentrations. The errors in results in table 1 are between 0.6 and 26 percent, and agree favorably with the estimated standard deviations.

The sensitivity of the method is sufficient for determining nuclide concentrations in the presence of higher concentrations of several other nuclides. This is illustrated in table 1 by samples 5 and 6 in which the ^{137}Cs represents only about 5 percent of the total activity.

To summarize, the method is an accurate, sensitive, and rapid means for the routine analysis of gamma-ray spectra of large numbers of low activity samples.

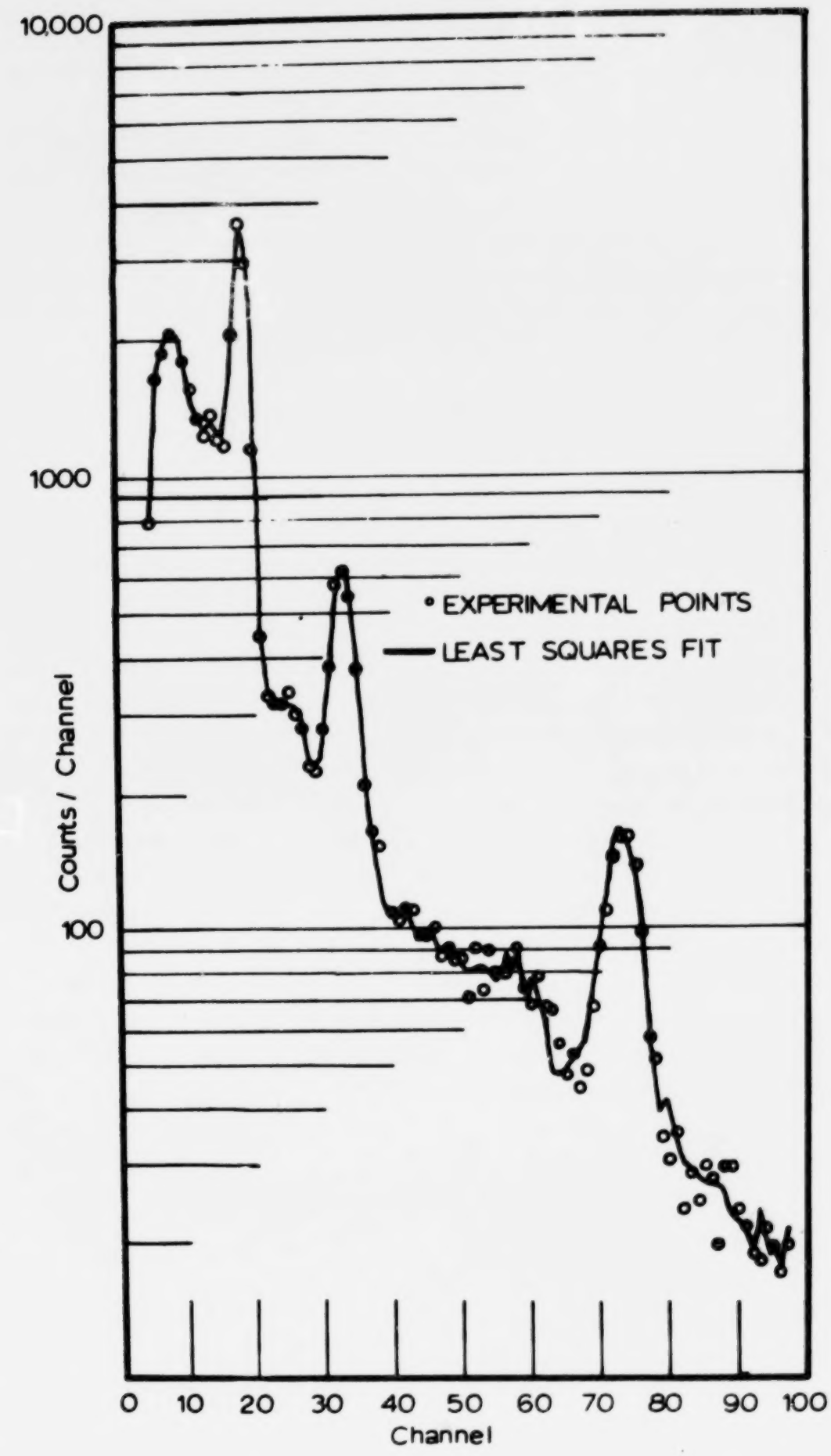

Figure 1. Analysis of a simulated milk sample containing ^{131}I, ^{137}Cs, and ^{40}K

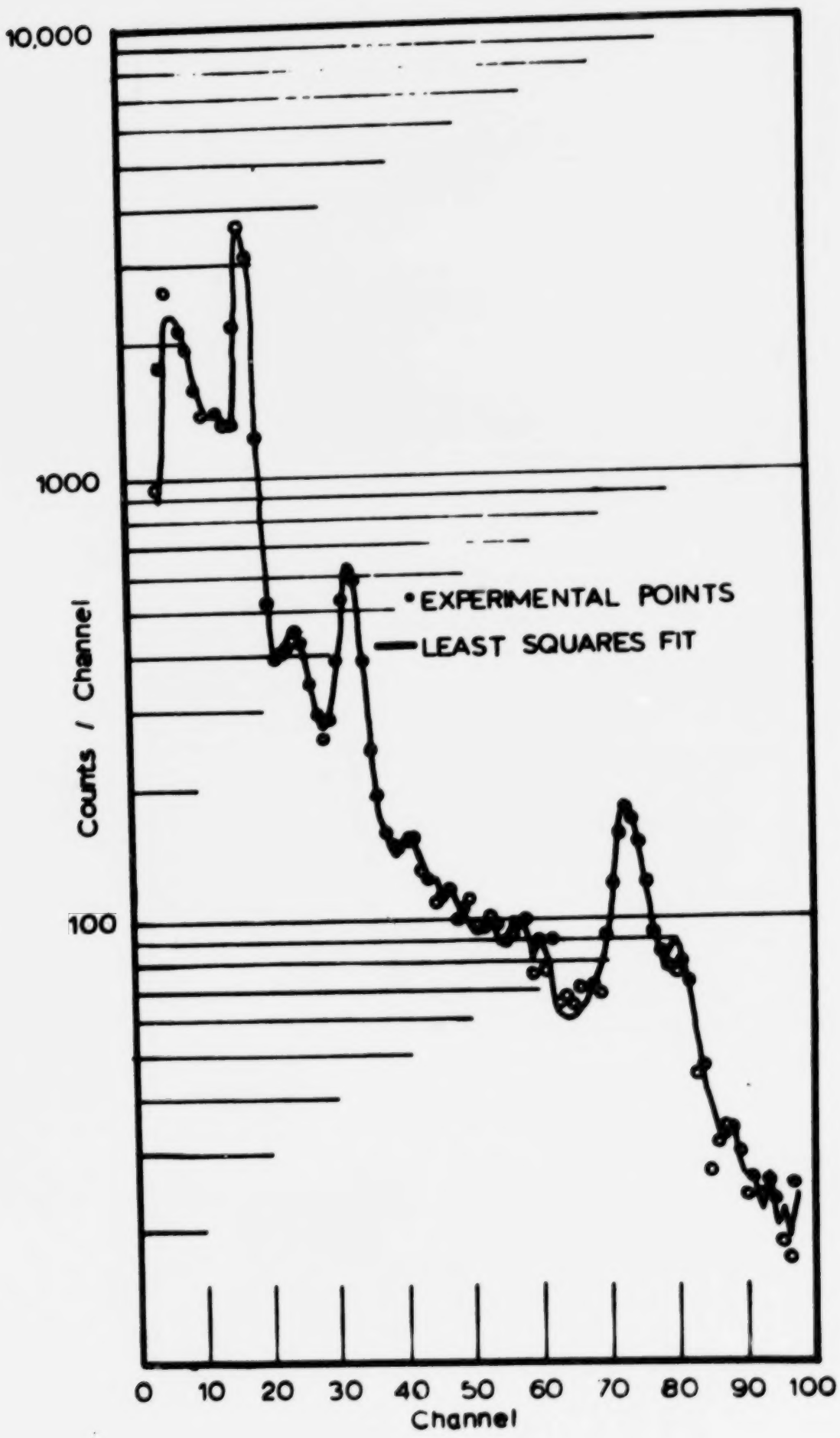

Figure 2. Analysis of a simulated milk sample containing ^{131}I, ^{137}Cs, ^{40}K, and ^{140}Ba-La

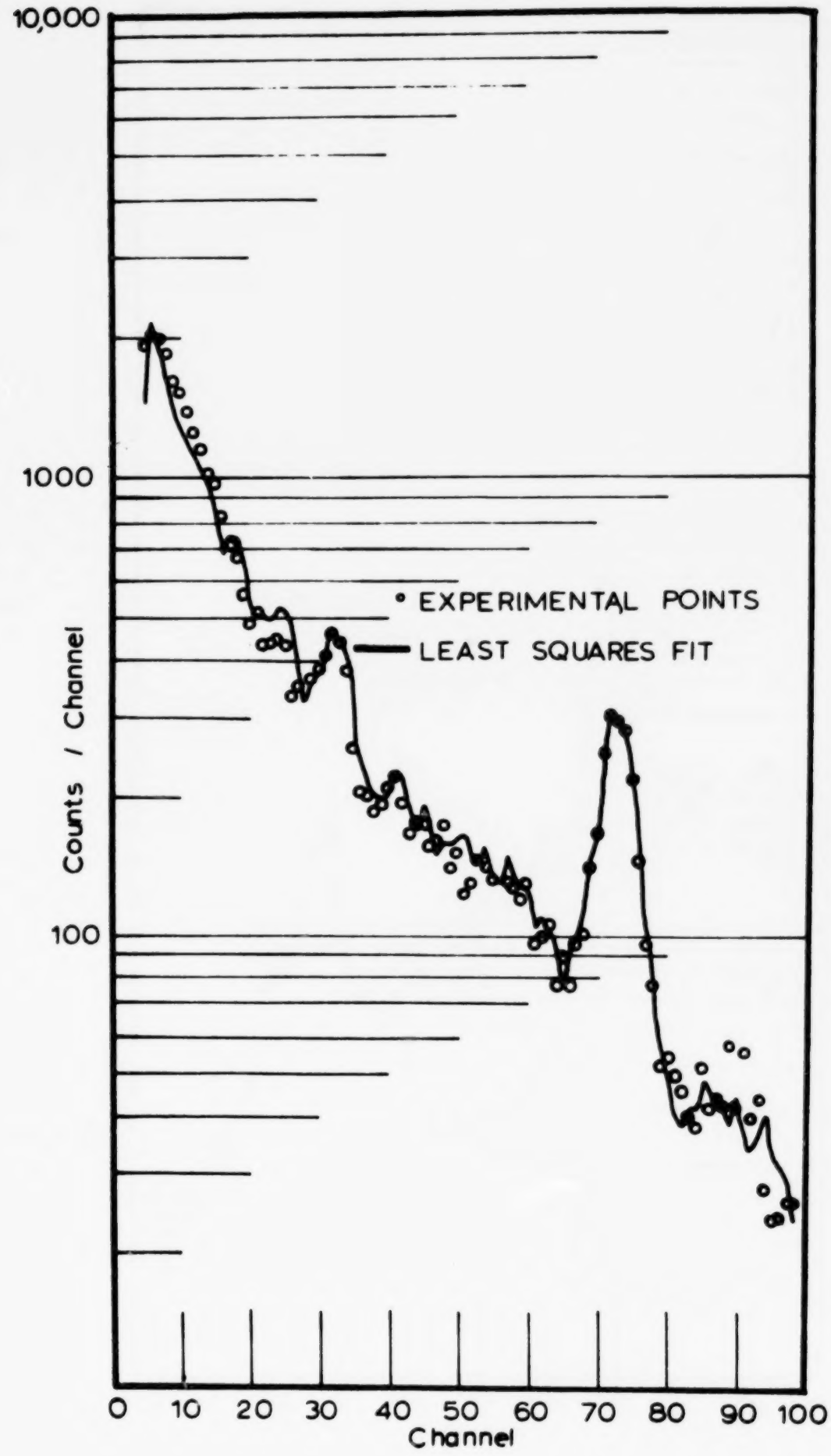

Figure 3. Analysis of a diet sample containing ^{137}Cs, ^{40}K, ^{144}Ce-Pr, and ^{54}Mn

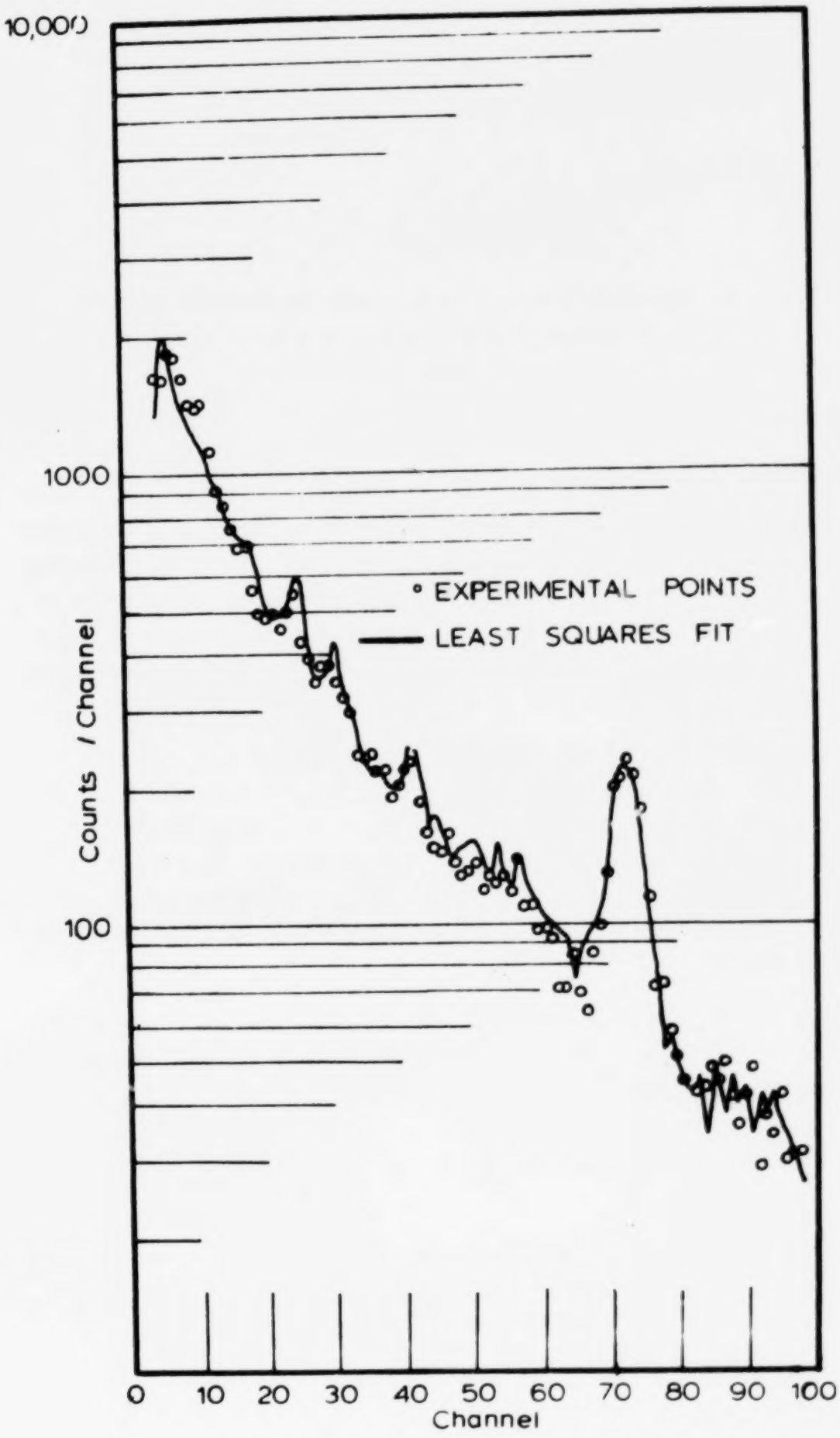

Figure 4. Analysis of a vegetation sample containing ^{40}K, ^{144}Ce-Pr, ^{54}Mn, and ^{106}Ru-Rh

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(*6*) HAGEE, G. R., G. J. KARCHES, and A. S. GOLDIN. Determi tion of I^{131}, Cs^{137}, and Ba^{140} in fluid milk by gamma sp troscopy. Talanta 5:36-43 (1960).

APPENDIX A

FORTRAN IV PROGRAM

Note: Considerable effort was expended to assure the accuracy of the program. It is hoped that all errors have been eliminated.

```
$IBFTC MAIN     DECK
C         GAMMA SPECTRA ANALYSIS BY METHOD OF LEAST SQUARES
C    PROGRAM SWITCHES NS1,NS2,ETC.  IN THE ON SETTING, THEY PRODUCE THE FOLLOWING
C  NS1....... ELIMINATES BACKGROUND AS A STANDARD
C  NS2....... ALLOWS RECALCULATION OF CONTRIBUTOR LIST AFTER L-S SOLUTION
C  NS3....... O M  ITS MATRIX APPROXIMATION
C  NS4....... ALLOWS OUTPUT AT THE END OF EACH ITERATION.
C  NS5....... ZEROES ANY NEGATIVE COUNTS (RESULTING FROM SUBTRACTING BACKGROUND)
C  NS6....... ALLOWS PUNCHING OF OBSERVED AND COMPUTED SPECTRUM WITH DIFFERENCE
       DIMENSION IPK(2,11), SAM(100), SXPK (13,13), SYPK(11  ),BKG(100),CONC(
      1  11), UNITS(11), STD(11,100), SAMP(100), YC(100), B(11), A(13,13), X(11)
      2  ,C(11), LIST(11 ), ISTP(11) , LSTSW(5), DC(11)
  100 READ 120,NSTDS,MINCH,MAXCH,KF ,MXIT,STIME  ,TOL ,BOUND,NS1,NS2,NS3
      1  ,NS4,NS5,NS6,NS7
  120 FORMAT (512,F4.0,F6.3,F4.1,711,12)
       PRINT121,NSTDS,MINCH,MAXCH,KF ,MXIT,STIME  ,TOL ,BOUND,NS1,NS2,NS3
      1  ,NS4,NS5,NS6
  121 FORMAT (1H1,512,F4.0,F6.3,F4.1,2X,611,5X,211,213,3X,15)
       IF (NS2.EQ.0.AND.NS4.EQ.0) GO TO 124
       CALL TYPE 1
       GO TO 125
  124 CALL TYPE 2
  125 NPTS=(MAXCH-MINCH+1)/KF
       READ 131,(LSTSW(I),I=1,5)
       READ 131,(IPK(1,I),IPK(2,I),I=1,NSTDS)
  131 FORMAT (30I2)
       KSTDS=NSTDS
  150 NSTDS=KSTDS
C  BEGIN READING AND STORING OF STANDARDS
       DO 190 J=1,NSTDS
       READ 151,NANL,ID,ID1,ID2,TIME,ND1,ND2,ND3,NHOU,MD1,MD2,MD3,KD1,
      1  KD2,DC(J),ISTP(J),CONC(J),UNITS(J),NUMBER
  151 FORMAT (2I1,I3,I3,3X,F3.0,3I2,I4,3I2,2I4,F9.7,A2,F10.1,A4,F4.0,I3)
       PRINT 152,NANL,ID,ID1,ID2,ISTP(J)
  152 FORMAT (1H ,2I1,2I3,3X,A2)
       READ 154,(SAM(I),I=1,100)
  154 FORMAT (11X,F5.0,3X,F5.0,3X,F5.0,3X,F5.0,3X,F5.0,3X,F5.0,3X,F5.0,
  1541  3X,F5.0,3X,F5.0 )
C  TEST FOR TIME BASE DIFFERENCE
       IF (STIME-TIME) 160,162,160
  160 CORREC=STIME/TIME
       DO 161 I=1,100
  161 SAM(I)=SAM(I)*CORREC
C  COMPRESS STANDARDS BY SPECIFIED COMPRESSION FACTOR (KF).
  162 DO 163 K=1,NPTS
       STD(J,K)=0.
       KK=K*KF+MINCH
       KKK=KK+KF-1
       DO 163 L=KK,KKK
  163 STD(J,K)=STD(J,K)+SAM(L)
C  TEST FOR BACKGROUND STANDARD
  172 IF (ID-4) 176,173,176
  173 DO 174 I=1,NPTS
  174 BKG(I)=STD(J,I)
       DO 171 I=1, 100
  171 YC(I)=SAM(I)
       CONC(J)=1.
       KBKG=J
       IF (NS1) 175,179,175
  175 KSTDS=NSTDS-1
```

```
      GO TO 150
C   SUBTRACT BACKGROUND FROM STANDARDS
  176 DO 177 I=1,NPTS
      STD(J,I)=STD(J,I)-BKG(I)
      IF (NS5) 1771,177,1771
 1771 IF (STD(J,I)) 1772,177,177
 1772 STD(J,I)=0.
  177 CONTINUE
      DO 178 I=1,100
  178 SAM(I)=SAM(I)-YC(I)
  179 IF (NS3) 190,180,190
C   SUM OVER SELECTED REGIONS FOR MATRIX APPROXIMATION
  180 DO 182 I=1,NSTDS
      LL1=IPK(1,I)
      LL2=IPK(2,I)
      SUM=0.
      DO 181 L=LL1,LL2
  181 SUM=SUM+SAM(L)
  182 SXPK(I,J)=SUM
  190 CONTINUE
      IF (NS3) 192,191,192
  191 CALL MATINV (SXPK,NSTDS)
C   BEGIN PROCESSING SAMPLES
  192 PRINT 195
  195 FORMAT (//10X,7HSAMPLES/)
      NSKIP=2
C  READ SAMPLE HEADER
  200 READ 151,NANL,ID,ID1,ID2,TIME,ND1,ND2,ND3,NHOU,MD1,MD2,MD3,KD1,
     1 KD2,SUM,IST,COOO,UNI,TD,NUMBER
      XNS7=NS2-1
      IF ((NANL+ID+ID1+ID2+ND1).EQ.0)  GO TO 100
      IF ((ID1-130).EQ.0)  GO TO 352
      KONTRL=0
      IF (NSKIP-9) 203,202,203
  202 KONTRL=1
      NSKIP=1
  203 PRINT 201,KONTRL,NANL,ID,ID1,ID2,NUMBER
  201 FORMAT (3I1,2I3,3X,I5)
      NSKIP=NSKIP+1
      READ 154, (SAM(I),I=1,100)
C   TEST FOR TIME BASE DIFFERENCE
      IF (STIME-TIME) 204,206,204
  204 CORREC=STIME/TIME
      DO 205 I=1,100
  205 SAM(I)=SAM(I)*CORREC
C   COMPRESS BY SPECIFIED COMPRESSION FACTOR
  206 DO 207 K=1,NPTS
      SAMP(K)=0.
      KK=K*KF-KF+MINCH
      KKK=KK+KF-1
      DO 207 L=KK,KKK
  207 SAMP(K)=SAMP(K)+SAM(L)
C   IS THIS A BACKGROUND READING
      IF (ID-4) 227,223,227
  223 DO 224 I=1,100
  224 BKG(I)=SAM (I)
      DO 222 I=1, NPTS
  222 YC(I)=SAMP(I)
      IF (NS1) 200,225,200
C   UPDATE BACKGROUND STANDARDS
```

```
  225 DO 226 I=1,NPTS
  226 STD(KBKG,I)=SAMP(I)
      GO TO 200
  227 IF (NS1) 230,239,230
  230 DO 232 I=1,100
  232 SAM(I)=SAM(I)-BKG(I)
      DO 236 I=1,NPTS
      SAMP(I)=SAMP(I)-YC(I)
      IF (NS5)  233,236,233
  233 IF (SAMP(I))  234,236,236
  234 SAMP(I)=0.
  236 CONTINUE
C  COMPUTE COUNTS IN TOTAL SPECTRUM
  239 SUM=0.
      DO 221 I=1,NPTS
  221 SUM=SUM+SAMP(I)
C  OPTIONAL BYPASS OF MATRIX APPROXIMATION AND CONTRIBUTOR LIST
      IF (NS3) 260,240,260
C  BEGIN MATRIX APPROXIMATION
  240 DO 246 I=1,NSTDS
      LL1=IPK(1,I)
      LL2=IPK(2,I)
      W=0.
      DO 244 L=LL1,LL2
  244 W=W+SAM(L)
  246 SYPK(I)  =W
      CALL MATAXB (SXPK,SYPK,C,NSTDS)
  247 DO 248 I=1,NSTDS
  248 SYPK(I)=C(I)*CONC(I)
      PRINT 332,( SYPK(I),UNITS(I),I=1,NSTDS)
  260 DO 262 I=1,NSTDS
  262 LIST(I)=1
      KSTDS=NSTDS
C  BEGIN LEAST SQUARE ANALYSIS
  300 IT=0
  301 KNT=0
      DO 309 I=1,NPTS
      Y=SAMP(I)
      IF (IT) 303,302,303
  302 IF (Y) 3022,3022,3021
 3021 W=1./Y
      GO TO 304
 3022 W=1.
      GO TO 304
  303 IF (YC(I)) 3031,3022,3031
 3031 W=1./YC(I)
  304 M=1
      DO308 J=1, NSTDS
      IF (LIST(J).EQ.0) GO TO 308
      X(M)=STD(J,I)
      M=M+1
  308 CONTINUE
      CALL NORMAL (X,KSTDS,Y,W,A,B,KNT,NPTS,LSTSW)
  309 CONTINUE
      KK=KSTDS+1
      DENOM=NPTS-KSTDS
      Y=A(KK,KK)
      R=Y/DENOM
C  CONSTRUCTION OF COMPUTED SPECTRUM
      DENOM=0.
```

```
      DO 311 I=1,NPTS
      YC(I)=0.
      M=1
      DO 310 J=1,NSTDS
      IF (LIST(J).EQ.0)  GO TO 310
      YC(I)=YC(I)+B(M)*STD(J,I)
      M=M+1
  310 CONTINUE
  311 DENOM=DENOM+YC(I)
      IF (TOL-R) 312,319,319
  312 IT =IT+1
C  OPTIONAL OUTPUT AFTER EACH ITERATION
  316 IF (MXIT-IT) 319,319,317
  317 IF (NS4) 318,301,318
  318 IJK=1
      GO TO 320
C  STATEMENT 319 IS THE NORMAL ENTRY TO OUTPUT REGION
  319 IJK=0
C  BEGIN OUTPUT REGION
  320 DO 321 I=1,KSTDS
  321 A( I,KK)=SQRT (A( I,KK))
      K=NSTDS
      KKK=KSTDS
  324 IF (LIST(K)) 326,325,326
  325 B(K)=0.
      A(K,KK)=0.
      GO TO 327
  326 B(K)=B(KKK)
      A(K,KK)=A(KKK,KK)
      KKK=KKK-1
  327 K=K-1
      IF (K-1) 328,324,324
  328 DO 322 I=1,NSTDS
      CORREC=EXP (TD*DC(I))
      A(I,KK)=A(I,KK)*CONC(I)*CORREC
  322 B(I)=B(I)*CONC(I)*CORREC
      IF (NSTDS-9) 330,330,333
  330 PRINT 331,(ISTP(I),I=1,NSTDS)
      PRINT 332,(B(I),UNITS(I),I=1,NSTDS)
      PRINT 332,(A(I,KK),UNITS(I),I=1,NSTDS)
  331 FORMAT (3X,A2,8(13X,A2))
  332 FORMAT (F7.3,,A1,8(F10.3,1X,A4))
      GO TO 334
  333 PRINT 331,(ISTP(I),I=1,9)
      PRINT 332,(B(I),UNITS(I),I=1,9)
      PRINT 332,(A(I,KK),UNITS(I),I=1,9)
  337 FORMAT (18X,6(A2,13X))
      PRINT 337, (ISTP(I),I=10,NSTDS)
      PRINT 336,(B(I),UNITS(I),I=10,NSTDS)
      PRINT 336,(A(I,KK),UNITS(I),I=10,NSTDS)
  336 FORMAT ( 10X,8(F10.3,1X,A4))
C  OUTPUT TOTAL SPECTRUM COUNTS, COMPUTED SPECTRUM TOTAL COUNTS, SUM OF
C    RESIDUALS SQUARED(WEIGHTED), CHI-SQUARE/(NPTS-NSTDS),SUM OF RESIDUALS
C    SQUARED (UNWEIGHTED).
  334  PRINT 335,SUM,DENOM,Y       ,R,A(KK,KSTDS+2)
  335  FORMAT (F12.0,F12.0,3E17.8)
C  OPTIONAL OUTPUT OF OBSERVED AND COMPUTED SPECTRUM WITH DIFFERENCES
      IF (NS6) 340,341,340
  340  PUNCH121,NSTDS,MINCH,MAXCH,KF ,MXIT,STIME  ,TOL ,BOUND,NS1,NS2,NS3
      1 ,NS4,NS5,NS6,    NAME,ID,ID1,ID2,NUMBER
```

```
  341 W=0.
      CORREC=0.
      DO 342 I=1,NPTS
      Y=SQRT (SAMP(I))
      DENOM=SAMP(I)-YC(I)
      R=DENOM/Y
      W=W+R
      CORREC=CORREC+R*R
      IF (NS6)  344,342,344
  344 PUNCH 343,I,SAMP(I),Y,YC(I),DENOM,R
  343 FORMAT (I3,F13.3,F10.3,F13.3,F11.3,F8.1)
  342 CONTINUE
      Y=NPTS
      W=W/Y
      CORREC=CORREC/Y
      PRINT 343,NPTS,W,CORREC
C   WAS ENTRY TO OUTPUT REGION BY PROGRAM SWITCH.  IF SO, RETURN TO INTERRUPTION
C     POINT.  IF NORMAL ENTRY, READ A NEW SAMPLE.
  350 IF (IJK)301,351,301
  351 IF ((XNS7.LT.0.).OR.(XNS7.EQ.3.)) GO TO 200
      KSTDS=NSTDS
      DO 356 I=1,NSTDS
      IF (B(I).LE.(A(I,KK)*XNS7))GO TO 355
      LIST(I)=1
      GO TO 356
  355 LIST(I)=0
      KSTDS=KSTDS-1
  356 CONTINUE
      XNS7=XNS7+1.
      PRINT 358
  358 FORMAT (/)
      GO TO 301
  352 END
```

APPENDIX B

FORTRAN IV PROGRAM SUBROUTINES

```
$IBFTC DECKY
C     SUBROUTINE NORMAL / USES MATINV(B,N)
C     FORMS AND SOLVES NORMAL EQUATIONS FOR MIN SUM W*(YO-YC)**2
C       WHERE W IS WEIGHT OF A GIVEN DATA POINT (YO,X(1),...X(N))
C     EQUATION OF CONDITION IS/ YC=A1*X1+A2*X2+...AN*XN
C     KNT SHOULD BE SET TO ZERO PRIOR TO FIRST ENTRY
C     WHEN KNT=NOPTS THE FOLLOWING RESULTS ARE RETURNED/
C    1)  SOLUTION VECTOR A(I),1=1,N
C    2)  VARIANCE OF A(1) IN B(I,N1)
C    3)  CORRELATION OF Y WITH X(I) IN B(I,N2)

C    5)  MEAN OF X(I) IN B(N2,I)
C    6)  STANDARD DEVIATION OF Y IN B(N2,N2)  MEAN Y IN B(N2, N1)
C    7)  SUM RESIDUALS SQUARED (WEIGHTED) IN B(N1,N1)
C    8)  SUM RESIDUALS SQUARED (UN WEIGHTED) IN B(N1,N2)
C     OPTIONAL OUTPUT IS CONTROLLED BY LSTSW (LIST SWITCHES)
C     LSTSW(I)=1 GIVES OUTPUT, =0 SUPPRESSES OUTPUT
C     LSTSW(1)/ B MATRIX COL. WISE BEFORE CALLING INVERSE
C     LSTSW(2)/ B MATRIX COL. WISE AFTER CALLING INVERSE
C     LSTSW(3)/ X(I) MEAN, STD.DEV., AND CORRELATION WITH Y
C     LSTSW(4)/ Y MEAN, STD. DEV. Y, AND SUM OF RESIDUALS SQUARED
C     LSTSW(5)/ A(I) COEFFICIENTS AND VARIANCES
      SUBROUTINE NORMAL(X,N,Y,W,B,A,KNT,NOPTS,LSTSW)
      DIMENSION X(11),B(13,13),A(11),LSTSW(5)
      IF(KNT) 1,1,2
 1    NM1=N-1
      N1=N+1
      N2=N+2
      FN=NOPTS
      FNMM=NOPTS-N
      DO 11 I=1,N2
      DO 11 J=1,N2
 11   B(I,J)=0.
 2    KNT=KNT+1
      DO 23 I=1,N
      T=X(I)
      WT=W*T
      B(I,N1)=B(I,N1)+WT*Y
      B(I,N2)=B(I,N2)+T*Y
      B(N2,I)=B(N2,I)+T
      B(N1,I)=B(N1,I)+T*T
      DO 23 J=I,N
 23   B(I,J)=B(I,J)+WT*X(J)
      T=Y*Y
      B(N1,N1)=B(N1,N )+W*T
      B(N1,N2)=B(N1,N2)+T
      B(N2,N2)=B(N2,N2)+Y
      IF(KNT-NOPTS) 60,30,30
C     MIRRORS ELEMENTS ACROSS THE DIAGONAL
 30   DO 31 I=1,NM1
      J1=I+1
      DO 31 J=J1,N
 31   B(J,I)=B(I,J)
      IF(LSTSW(1)) 32,33,32
 32   PRINT 200,((B(I,J),I=1,N2),J=1,N2)
 200  FORMAT(2H01,3X,5F15.8)
 33   CALL MATINV(B,N)
      DO 41 I=1,N
      T=0.
      DO 40  J=1,N
```

```
   40   T=T+B(I,J)*B(J,N1)
   41   A(I)=T
C       COMPUTES SUM SQUARES, STANDARD DEVIATIONS, AND CORRELATION COEFF.
        SSQ=B(N1,N2)
        SSQW=B(N1,N1)
        YBAR=B(N2,N2)/FN
        B(N2,N1)=YBAR
        STDVY=SQRT (SSQ/FN-YBAR*YBAR)
        B(N2,N2)=STDVY
        DO 50 I=1,N
        XBAR=B(N2,I)/FN
        B(N2,I)=XBAR
        STDVX=SQRT (B(N1,I)/FN-XBAR*XBAR)
        B(N1,I)=STDVX
        SUMXY=B(I,N2)
        IF(STDVX)48,47,48
   47   B(I,N2)=0.
        GO TO 49
   48   B(I,N2)=(SUMXY/FN-XBAR*YBAR)/(STDVX*STDVY)
   49   T=A(I)
        SSQ=SSQ-T*SUMXY
   50   SSQW=SSQW-T*B(I,N1)
        B(N1,N1)=SSQW
        B(N1,N2)=SSQ
        T=SSQW/FNMM
        DO 510I=1,N
  510   B(I,N1)=T*B(I,I)
        IF(LSTSW(2)) 51,52,51
   51   PRINT 200,((B(I,J),I=1,N2),J=1,N2)
   52   IF(LSTSW(3)) 53,54,53
   53   DO 530 I=1,N
  530   PRINT 201,I,B(N2,I),B(N1,I),B(I,N2)
  201   FORMAT(2HO1,2HX(,12,3H)  ,5HMEAN=E14.8,2X,9HSTD.DEV.=E14.8,2X,
        19HCORR.W/Y=E14.8)
   54   IF(LSTSW(4)) 55,56,55
   55   PRINT 202,B(N2,N1),B(N2,N2)
  202   FORMAT(2HO1,10HMEAN OF Y=E16.8,5X,15HSTAND.DEV.OF Y=E16.8)
        PRINT 203,B(N1,N1),B(N1,N2)
  203   FORMAT(2HO1,13HSUM of SQRS.=E16.8,5X,17HSUM of SQRS.WTD.=E16.8)
   56   IF(LSTSW(5)) 57,60,57
   57   DO 570 I=1,N
  570   PRINT 204,I,A(I),B(I,N1)
  204   FORMAT(2HO1,3X,2HA(,12,2H)=E16.8,5X,9HVARIANCE=E16.8)
   60   RETURN
        END
```

```
$IBFTC DECKZ
C       INVERTS MATRIX A BY CHOLESKI METHOD
        SUBROUTINE MATINV(A,N)
        DIMENSION A(13,13)
        NM1=N-1
        NP2=N+2
        DO 10 IP=2,N
        IRLIM=IP-1
        DO 20 IR=1,IRLIM
        ISLIM=IR-1
        SUM=A(IP,IR)
        IF(ISLIM)23,23,21
   21   DO 22 IS=1,ISLIM
   22   SUM=SUM-A(IP,IS)*A(IS,IR)
   23   A(IP,IR)=SUM/A(IR,IR)
   20   CONTINUE
        DO 10 IR=IP,N
        ISLIM=IP-1
        SUM=A(IP,IR)
        DO 30 IS=1,ISLIM
   30   SUM=SUM-A(IP,IS)*A(IS,IR)
        A(IP,IR)=SUM
   10   CONTINUE
C       COMPUTE INVERSE OF LOWER TRING B AND STORE IN C
        DO 40 J=1,NM1
        I1=J+1
        DO 40 I=I1,N
        SUM=-A(I,J)
        K1=J+1
        KLIM=I-1
        IF(KLIM-K1)51,49,49
   49   DO 50 K=K1,KLIM
   50   SUM=SUM-A(I,K)*A(K,J)
   51   A(I,J)=SUM
   40   CONTINUE
C       COMPUTE INVERSE OF UPPER TRIANG T AND STORE IN D
        DO 60 I=1,N
   60   A(I,I)=1./A(I,I)
        DO 70 JX=2,N
        J=NP2-JX
        IXLIM=J-1
        DO 70 IX=1,IXLIM
        I=J-IX
        K1=I+1
        KLIM=J
        SUM=0.
        DO 61 K=K1,KLIM
   61   SUM=SUM+A(I,K)*A(K,J)
        A(I,J)=-A(I,I)*SUM
   70   CONTINUE
C       COMPUTE INVERSE OF A = D.C. AND STORE IN A
        DO 80 I=1,N
        DO 80 J=1,N
        SUM=0.
        DO 90 M= 1,N
        IF(M-I) 90,91,91
   91   IF(M-J)90,92,93
   92   SUM=SUM+A(I,M)
        GO TO 90
   93   SUM=SUM+A(I,M)*A(M,J)
```

```
90  CONTINUE
    A(I,J)=SUM
80  CONTINUE
95  RETURN
    END
```

```
    SUBROUTINE MATAXB (A,B,C,N)
    DIMENSION A(13,13),B(11),C(11)
    DO 10 I=1,N
    C(I)=0.
    DO 10 J=1,N
10  C(I)=C(I)+B(J)*A(I,J)
    RETURN
    END
```

(Note: The following program applies only to machine with 1401 on line.)

```
$IBMAP  DECKW
        ENTRY   TYPE1
        ENTRY   TYPE2
MES1    BCI     8,SET 1401 SWITCHES TO SUPRESS CARRIAGE CONTROL
MES2    BCI     8,SET 1401 SWITCHES FOR PROGRAM CARRIAGE CONTROL
TYPE1   TRA     **
        TSX     S.XPRT,4
        PZE     MES1,,45
        HPR
        TRA     TYPE1
TYPE2   TRA     **
        TSX     S.XPRT,4
        PZE     MES2,,46
        HPR
        TRA     TYPE2
        END
```

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